Nanoscale Fabrication of Mesoscale Objects

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Neither LLNL nor any other organization has the capability to perform deterministic fabrication of mm-sized objects with arbitrary, μm-sized, 3-D features and with 20-nm-scale accuracy and smoothness. This is particularly true for materials such as high explosives and low-density aerogels.

In this project, we have, for the first time, combined the 1-D hydrocode "HYADES" with the 3-D molecular dynamics simulator "MDCASK" in our modeling studies. In FY2002 and FY2003, we investigated the ablation/surface-modification processes that occur on copper, gold, and nickel substrates with the use of sub-ps laser pulses. In FY2004, we investigated laser ablation of carbon, including laser-enhanced chemical reaction on the carbon surface for both vitreous carbon and carbon aerogels.

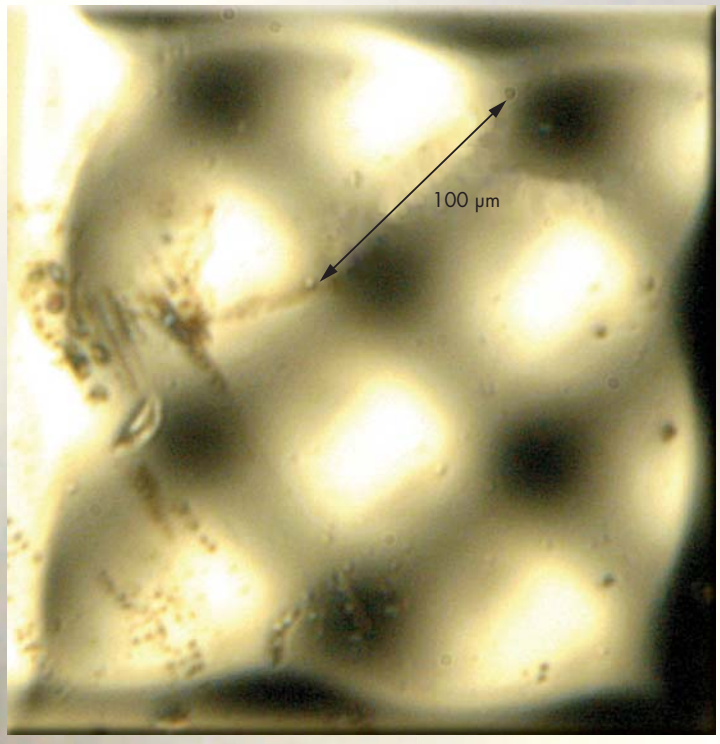

Figure 1. Optical micrograph of sinusoidal moguls, micromachined on vitreous carbon using reactive (oxygen) ion-beam milling.

Project Goals

The immediate impact of our investigation will be a much better understanding of the chemical and physical processes that influence materials that are exposed to fs laser pulses. More broadly, our goals are to develop the capability for fabricating and characterizing mesoscale objects using fs laser pulses and ion-beam etching for applications such as fabricating laser targets, developing miniature fuels cell, remote sensors, and medical technologies.

Relevance to LLNL Mission

These experiments will support the Laboratory's stockpile stewardship mission by providing data for corroborating the models in the improved physics codes for the Advanced Simulation and Computing Program, and developing new capabilities for the fabrication and characterization of mesoscale objects with nanoscale precision.

FY2004 Accomplishments and Results

In FY2004, using carbon substrates, we investigated the ablation processes that occur with the use of laser pulses to ablate the surface. We studied the process both in vacuum and in air. Our main effort used vitreous carbon, both

because it is readily available and because it was the easiest carbon to model. Through our collaboration with colleagues at Lawrence Berkeley Laboratory, we also showed that oxygen-ion beams could micromachine smooth features in vitreous carbon. We also studied laser ablation of carbon aerogels and were able to micromachine simple features in these aerogels. We submitted a manuscript to *Science* on our work on laser ablation of metals.

Figure 1 shows a vitreous-carbon sample with μm features. Figure 2 shows metrology plots for that sample.

Related References

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2. Mariella, R. P., Jr., "MEMS-Based Sensor Systems," *NNSA Futures Conference,* Crystal City, Virginia, May 2004.
3. Gilmer, G. H., M. D. Shirk, A. M. Rubenchik, L. Zepeda-Ruiz, R. P. Mariella, Jr., T. Diaz de la Rubia, "Short-Pulse Laser Ablation Simulated by Molecular Dynamics, Void Nucleation and Cluster Ejection," *Third International Conference: Computational Modeling and Simulation of Materials,* Acireale, Sicily, Italy, May 30-June 4, 2004.
4. Gilmer, G. H., "Thin Film Deposition and Manipulation of Surfaces Using Laser Beams: Atomistic Modeling," *DOE-NSET Workshop on Artificially Structured Nanomaterials: Formation and Properties,* Gatlinburg, Tennessee, October 13-15, 2003.
5. Gilmer, G. H., "Short-Pulse Laser Ablation of Metals: Large-Scale Molecular Dynamics Simulations," *Second International Workshop on Strength and Fracture,* Berkeley, California, January 7-9, 2004.

FY2005 Proposed Work

We have made numerous interesting discoveries that merit further work. The ability to contour difficult materials needs to be placed into a more deterministic framework. That is, the quantitative relationship between the nominal fluence of the laser pulses and the micromachining needs to be better characterized, particularly in terms of the effect of pulse-to-pulse variability with variability in amount of material removed, and in the 3-D shape of the feature that is created in the substrate. Both chemically-assisted laser ablation as well as reactive-ion-beam etching of carbon warrant further investigations. For microfabricating 3-D objects of diamond, traditional machining will be ineffective, and lasers and ion beams will be the clear methods of choice. Diamond is being considered, for example, as a material that could serve as the ignition capsule on NIF.

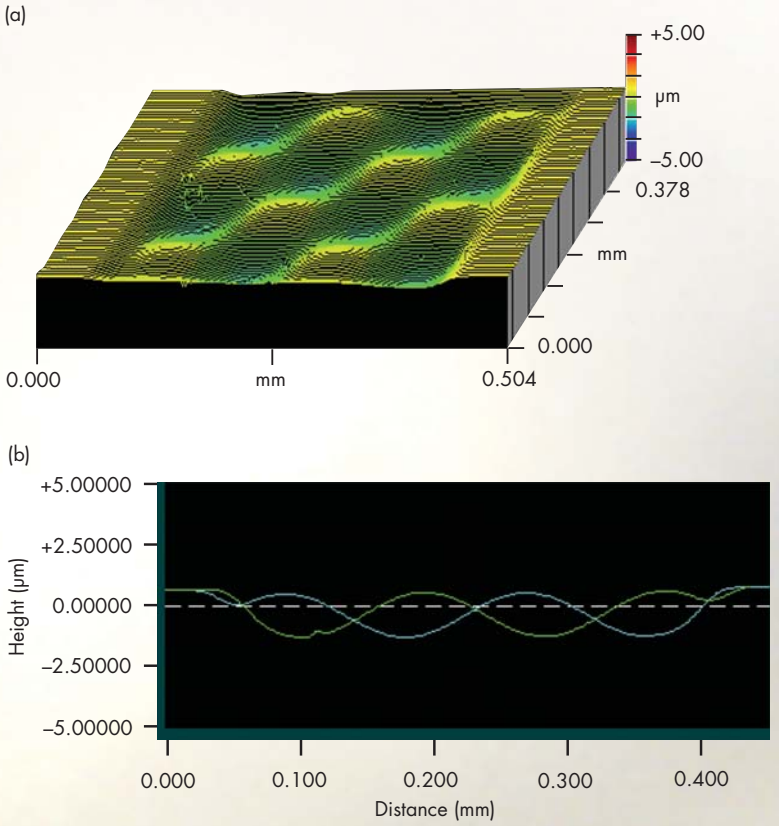

Figure 2. Optical-profilometer (a) image and (b) line scans of sinusoidal moguls, micromachined in the carbon substrate of Fig. 1.